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The Revival of Active Set Methods

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1. Why Do We Need Active Set Methods?

2. Active Set Methods for Quadratic Programs

3. Active Set Methods for Nonlinear Programs

Why Do We Need Active Set Methods (ASMs)?

Philosophy
Lesson

Issues in Optimization Solvers

$$\underset{x}{\text{minimize}}\; f(x) \qquad \text{subject to}\; c(x) \geq 0$$

1. **Global Convergence**
2. **Active Set Identification**
3. **Fast Local Convergence**

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$$\underset{x}{\text{minimize}}\ f(x) \qquad \text{subject to}\ c(x) \geq 0$$

1. **Global Convergence**
   - merit function, e.g. $f(x) + \pi \| c(x)^- \|$ for $\pi > \| y^* \|_D$
   - filter ... more later
2. **Active Set Identification**
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   - given active set, simply use Newton's method
   - step computation: update estimate of active set
   - alternative: interior point methods $Yc(x) = \mu e$ & $\mu \searrow 0$
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3. **Fast Local Convergence**
   - conjugate gradients et al.
   - (constrained) preconditioners

Why Do We Need Active Set Methods (ASMs)?

Interior point methods (IPMs) usually faster than ASMs:

1. Pivoting inefficient for huge problems
2. Single QP solve $\simeq$ several Newton steps of IPM
3. Null-space projected Hessian factors are **DENSE**

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Why should we be interested in ASMs?

- ASMs often more robust than interior point methods
- ASMs better for warm-starts (repeated solves)
- Easier to precondition ... iterative solves

Challenge: overcome 1. & 2. from above

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Two ways to make large changes to active set

1. Projected gradient approach
2. Sequential linear programming approach

ACTIVE SET METHODS FOR QPs

Active Sets for Quadratic Programs (QPs)

$$\boxed{\begin{array}{ll} \underset{x}{\text{minimize}} & \frac{1}{2}x^T H x + g^T x \\ \text{subject to} & A^T x = b \\ & l \le x \le u \end{array}}$$

- H is symmetric (indefinite?)
- A^T is $m \times n$, $m < n$, full rank
- General: $\bar{l} \le \begin{pmatrix} x \\ A^T x \end{pmatrix} \le \bar{u}$

$$\begin{array}{ll} \text{Active set} & \mathcal{A}(x) = \{i \mid x_i = l_i \text{ or } x_i = u_i\} \\ \text{Inactive set} & \mathcal{I}(x) = \{1, \ldots, n\} - \mathcal{A}(x) \end{array}$$

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Given $\mathcal{A}$, QP solution $(x^*_{\mathcal{I}}, y^*)$ solves

$$\begin{bmatrix} H_{\mathcal{I},\mathcal{I}} & -A_{:,\mathcal{I}} \\ A^T_{:,\mathcal{I}} & \end{bmatrix} \begin{pmatrix} x_{\mathcal{I}} \\ y \end{pmatrix} = \begin{pmatrix} -g_{\mathcal{I}} - H_{\mathcal{I},\mathcal{A}} x_{\mathcal{A}} \\ b - A^T_{:,\mathcal{A}} x_{\mathcal{A}} \end{pmatrix}$$

Active-set methods search for $\mathcal{A}^*$:

- Delete entries from $\mathcal{A}^k$; update a factorization; compute step
- Possibly add entries to $\mathcal{A}^k$
- $\exists$ robust solvers; good for warm starts ... n large ???

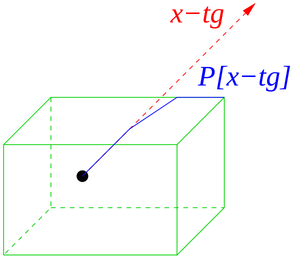
PROJECTED GRADIENT

Projected Gradient for Box Constrained QPs

Simpler box constrained QP ...

$$\left\{ \begin{array}{ll} \underset{x}{\text{minimize}} & \frac{1}{2}x^THx + g^Tx \; =: \; q(x) \\ \text{subject to} & l \le x \le u \end{array} \right.$$

Projected steepest descent $P[x - \alpha \nabla q(x)]$
○ piecewise linear path
... large changes to $\mathcal{A}$-set
... but slow (steepest descent)



x^c Cauchy point $\equiv$ first minimum of $q(x(\alpha))$, for $\alpha \ge 0$

Theorem: Cauchy points converge to stationary point.

Projected Gradient & CG for Box Constrained QPs

```
$x^0$ given such that $l \le x^0 \le u$; set $k = 0$
WHILE (not optimal) BEGIN
    1. find Cauchy point $x_k^c$ & active set $\mathcal{A}(x_k^c)$
    2. (approx.) solve box QP in subspace $\mathcal{I} := \{1, \ldots, n\} - \mathcal{A}(x_k^c)$
       $\boxed{\begin{array}{ll} \underset{x}{\text{minimize}} & \frac{1}{2}x^T Hx + g^T x \\ \text{subject to} & l \le x \le u \\ & x_i = [x_k^c]_i \; , \forall \; i \in \mathcal{A}(x_k^c) \end{array}} \Leftrightarrow \boxed{\begin{array}{l} \text{apply CG to ...} \\ H_{\mathcal{I},\mathcal{I}} x_{\mathcal{I}} = \ldots \end{array}}$
       for $x^{k+1}$; set $k = k + 1$
END
```

Cauchy point $\Rightarrow$ global convergence ... but faster due to CG

How to Include $A^T x = b$?

Projection onto box is easy, but tough for general QP

$$P_{QP}[z] = \left\{ \begin{array}{ll} \underset{x}{\text{minimize}} & (x-z)^T(x-z) \\ \text{subject to} & A^T x = b \\ & l \leq x \leq u \end{array} \right.$$

... as hard as original QP! ... Idea: project onto box only

$\Rightarrow$ subspace solve $H_{\mathcal{I},\mathcal{I}} x_{\mathcal{I}} = \dots$ becomes solve with KKT system

$$\begin{bmatrix} H_{\mathcal{I},\mathcal{I}} & -A_{:,\mathcal{I}} \\ A^T_{:,\mathcal{I}} & \end{bmatrix} \begin{pmatrix} x_{\mathcal{I}} \\ y \end{pmatrix} = \dots$$

Which gradient / merit function in Cauchy step?

AUGMENTED LAGRANGIAN

The Augmented Lagrangian

Arrow & Solow ('58), **Hestenes** ('69), **Powell** ('69)

$$\boxed{\underset{x}{\text{minimize}}\ L(x, y_k, \rho_k) \ = \ f(x) - y_k^T c(x) + \tfrac{1}{2}\rho_k \|c(x)\|^2}$$

As $y_k \to y_*$:
- $x_k \to x_*$ for $\rho_k > \bar{\rho}$
- No ill-conditioning, improves convergence rate

- An old idea for nonlinear constraints ... smooth merit function
- Poor experience with LPs (e.g., MINOS vs. LANCELOT)
- But special structure of LPs (and QPs) not fully exploited

$$\boxed{f(x) = \tfrac{1}{2}x^T Hx + g^T x \quad \& \quad c(x) = A^T x - b}$$

Bound Constrained Lagrangian (BCL)

Minimizing the augmented Lagrangian subject to bounds:

WHILE (not optimal) **BEGIN**

1. Find $\omega_k \searrow 0$ optimal x_k of

$$\boxed{\underset{l \le x \le u}{\text{minimize}} \quad f(x) - y_k^T c(x) + \frac{1}{2}\rho_k \|c(x)\|^2}$$

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  2. IF $\|c(x_k)\| \le \eta_k \searrow 0$ THEN
         Update $y_k$ ( typically $y_{k+1} = y_k - \rho_k c(x_k)$ )
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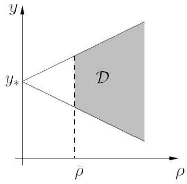
Arbitrary sequences: $\eta_k \& \omega_k$ control feasibility & optimality

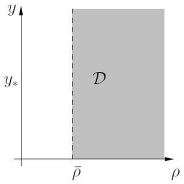
Augmented Lagrangian for Linear Constraints

Nonlinear $c(x)$



$(y_k, \rho_k) \in \mathcal{D}$

$c(x) = A^T x - b$



$\rho_k > \bar{\rho}$

$\forall (\rho, y) \in \mathcal{D}$, minimize $L(x, y, \rho)$ has unique solution $x(y, \rho)$:

- bound constrained augmented Lagrangian converges
- Hessian $\nabla^2_{xx} L(x, y, \rho)$ is positive definite on optimal face

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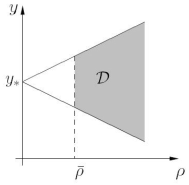

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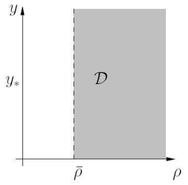

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$$\boxed{\bar\rho \approx 2 \frac{\|H_*\|}{\|A_* A^T{}_*\|}}$$ ... depends on active set ... from dual Hessian

QP by Projected Augmented Lagrangian QPPAL

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       $\boxed{\underset{l \le x \le u}{\text{minimize}} \; \frac{1}{2}x^T Hx + g^T x - y^T(A^T x - b) + \frac{1}{2}\rho_k \|A^T x - b\|^2}$
    2. Find $\mathcal{A}(x_k^c)$ & estimate penalty $\bar{\rho} = 2\,\|H_{\mathcal{I}}\|/\|A_{\mathcal{I}} A_{\mathcal{I}}^T\|$
    3. IF $\bar{\rho} > \rho_k$ THEN update $\rho_{k+1} = \bar{\rho}$ & CYCLE
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    5. Line-search on $L(x_k^c + \alpha\Delta x, y_k^c + \alpha\Delta y, \rho)$; update $x, y, k, \rho$
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1.-3. identify active set ... 4. gives fast convergence

Filter Methods

A Filter for Augmented Lagrangian Methods

Two competing aims in augmented Lagrangian:

1. reduce $h_k := \|A^T x_k - b\| \le \eta_k \searrow 0$
2. reduce $\theta_k := \|\nabla L(x_k, y_k, \rho_k) - z_k\| \le \omega_k \searrow 0$

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... why should one sequence $\{\omega_k\}, \{\eta_k\}$ fit *all problems ???*

A Filter for Augmented Lagrangian Methods

Introduce a filter $\mathcal{F}$ to promote convergence

- list of pairs $(\|A^T x_l - b\|, \|\nabla L_l - z_l\|)$
- no pair dominates any other pair
- new x_k acceptable to filter $\mathcal{F}$, iff
    1. $h_k \leq 0.99 \cdot h_l \; \forall l \in \mathcal{F}$
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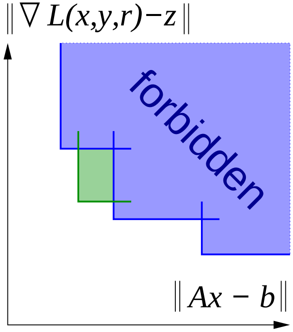

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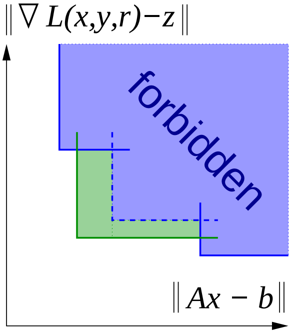

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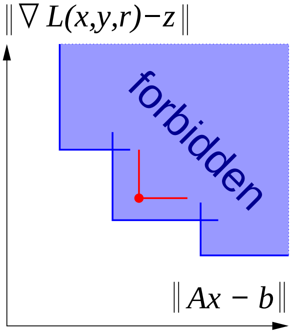

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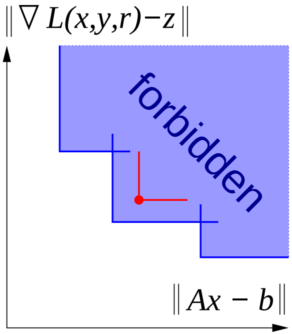

... and old friend from Chicago ...

Augmented Lagrangian Cauchy Pointe (Al Capone)

Requirement on Cauchy Point x_k^c for filter:

1. x_k^c, y_k^c acceptable to filter

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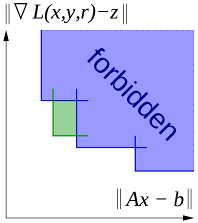
   ... optimality of Lagrangian



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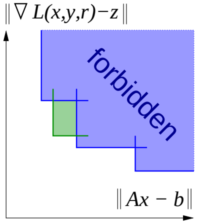
   ... depends on filter



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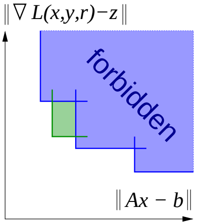

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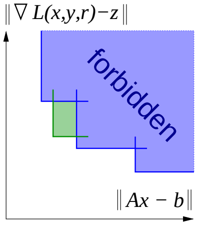

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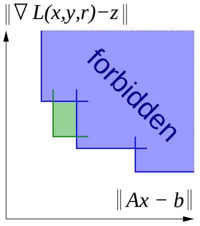
   ... if not acceptable then reduce $\omega_{k+1} = \omega_k/2$
2. & $\omega_{k+1} = \omega_k/2$ ensure new entry can be added to filter

Augmented Lagrangian Cauchy Pointe (Al Capone)

Requirement on Cauchy Point x_k^c for filter:

1. x_k^c, y_k^c acceptable to filter
2. $\|\nabla L(x_k, y_k, \rho_k) - z_k\| \leq \omega_k$
   ... optimality of Lagrangian

   New: $\omega_k := 0.1 \max\{\|\nabla L_l - z_l\|\}$
   ... depends on filter

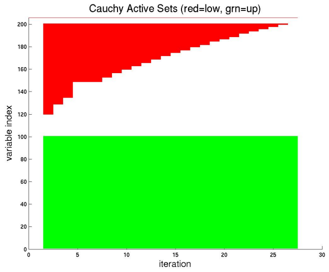


1. ensures that back-tracking line-search will succeed
   ... if not acceptable then reduce $\omega_{k+1} = \omega_k/2$
2. & $\omega_{k+1} = \omega_k/2$ ensure new entry can be added to filter

Why do you keep the penalty parameter?
... combines search directions for $\|A^T x - b\|$, and
$\|\nabla L(x_l, y_l, \rho_l) - z_l\|$
$\Rightarrow$ gradient projection possible

Active Set Evolution: `blockqp4_100`

AUGLAG

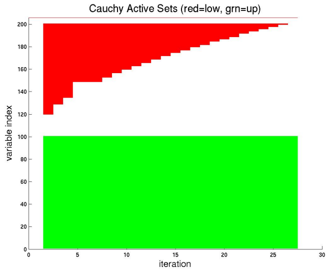


red = lower bound active

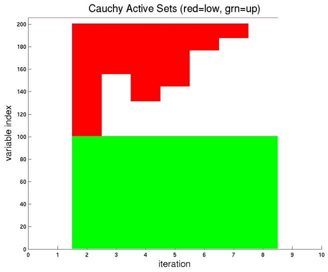
green = upper bound active

Active Set Evolution: `blockqp4_100`

AUGLAG



FILTER



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Summary: Active Set QP Method

1. **Global Convergence**

2. **Active Set Identification**

3. **Fast Local Convergence**

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     $\Rightarrow$ no arbitrary parameters
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   - conjugate gradients on equality QP
   - (constrained) preconditioners ???
   - Benzi-Golub ... ties in with augmented Lagrangian

ACTIVE SET METHODS FOR NLPs

Sequential Quadratic Programming (SQP)

$$\text{NLP:} \qquad \underset{x}{\text{minimize}} \; f(x) \qquad \text{subject to } \; c(x) \geq 0$$

SQP method of choice for NLP

Compute displacement/step d by solving QP subproblem

$$\boxed{\begin{array}{lll} \underset{d}{\text{minimize}} & g^T d + \frac{1}{2} d^T W d & \\ \text{subject to} & c + A^T d \geq 0 & \\ & \|d\|_\infty \leq \Delta & \text{Trust-Region} \end{array}}$$

where $g = \nabla f(x)$, $A = \nabla c(x)^T$, $W = \nabla^2 \mathcal{L}(x, y)$

Sequential Quadratic Programming (SQP)

```
WHILE (not optimal) BEGIN
  1. Compute displacement/step $d$ by solving QP subproblem
  2. IF step $d$ acceptable THEN
           $x = x + d$ & increase trust-region radius $\Delta = 2 * \Delta$
     ELSE
           $x = x$ & decrease trust-region radius $\Delta = \Delta/2$
END
```

- How to make it work for *n* large ???
  QP solve is bottleneck ... could use new QPFIL
- $\exists$ excellent LP solvers ... but QP harder

Sequential Linear Programming

Throw away quadratic term $\Rightarrow$ linear program

Compute displacement/step d_{LP} by solving LP subproblem

$$\boxed{\begin{array}{lll} \underset{d}{\text{minimize}} & g^T d + \frac{1}{2} d^T W d & \\ \text{subject to} & c + A^T d \geq 0 & \\ & \|d\|_\infty \leq \Delta & \text{Trust-Region} \end{array}}$$

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END
```

$\Rightarrow$ slow local convergence ... steepest descent

Sequential Linear Programming

```
WHILE (not optimal) BEGIN
    1. Compute displacement/step $d_{LP}$ by solving LP subproblem
    2. Identify active constraints: $\mathcal{A} = \{i : c_i + a_i^T d_{LP} = 0\}$ & solve
```

$$\begin{array}{lll} \underset{d}{\text{minimize}} & g^T d + \frac{1}{2} d^T W d & \\ \text{subject to} & c_i + a_i^T d = 0 & i \in \mathcal{A} \end{array} \Leftrightarrow \begin{bmatrix} H_{\mathcal{I},\mathcal{I}} & -A_{:,\mathcal{I}}^T \\ A_{:,\mathcal{I}} & \end{bmatrix} \left(\begin{array}{c} d_{\mathcal{I}} \\ y \end{array} \right.$$

```
       equality QP for step $d$
    3. IF step $d$ acceptable THEN
            $x = x + d$ & increase trust-region radius $\Delta = 2 * \Delta$
       ELSE
            $x = x$ & decrease trust-region radius $\Delta = \Delta/2$
END
```

How expensive are LPs??

Active Set Identification by SLP

Polyhedral trust-region makes LP solves inefficient

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- many changes to active trust-region bounds
- LP solvers too slow near solution

Active Set Identification by SLP

Ellipsoidal trust-region makes LPs into NLPs

$$\boxed{\begin{array}{lll} \underset{d}{\text{minimize}} & g^T d & \\ \text{subject to} & c + A^T d \geq 0 & \\ & \|d\|_2 \leq \Delta & \text{Trust-Region} \end{array}}$$

- trust-region (always) active $\Rightarrow$ no changes
- subproblem is now NLP ... as hard as original problem ???

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Ellipsoidal trust-region makes LPs into NLPs

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